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**COMPUTATIONAL TECHNIQUES FOR
FLOWS WITH FINITE-RATE CONDENSATION**

Submitted By:

Graham V. Candler*
Principal Investigator
Department of Aerospace Engineering and Mechanics
University of Minnesota
Minneapolis MN 55455
612-625-2364 Fax: 612-626-1558

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* Previous address: Mechanical and Aerospace Engineering Department, North Carolina State University, Raleigh NC 27695-7921

FINAL REPORT

Introduction

A computational method to simulate the inviscid two-dimensional flow of a two-phase fluid has been developed. This computational technique treats the gas phase and each of a prescribed number of particle sizes as separate fluids which are allowed to interact with one another. Thus, each particle-size class is allowed to move through the fluid at its own velocity at each point in the flow field. Mass, momentum, and energy are exchanged between each particle class and the gas phase. It is assumed that the particles do not collide with one another, so that there is no inter-particle exchange of momentum and energy. However, the particles are allowed to grow, and therefore, they may change from one size class to another. Appropriate rates of mass, momentum, and energy exchange between the gas and particle phases and between the different particle classes have been developed. A numerical method has been developed for use with this equation set. Several test cases have been computed and show qualitative agreement with previous calculations. This work has been reported at the 1993 AIAA Aerospace Sciences Meeting in Reno NV. A copy of the conference paper is enclosed¹. A summary of the results of the research follows and more details may be found in the attached paper.

Combustion-driven hypersonic wind tunnels have a test gas that has a significant mass fraction of water in either vapor or condensed form. The presence of water droplets can affect the performance of the nozzle and the behavior of the gas in the test section. A quasi-one-dimensional numerical method to simulate these flows has been developed at NASA Langley by Erickson *et al*². Results from this code show significant increases in the test section static pressure and entropy over that obtained for an ideal nozzle expansion. The research used this work as a starting point for the development of a two-dimensional computational fluid dynamics algorithm. Additional recent work of interest was performed by Elangovan and Cao³, in which they modeled dusty supersonic viscous flows. This work demonstrates that CFD methods can be used to simulate flows with suspended particles, such as flows with condensation. The research used a combination of these approaches to develop a computational method for the simulation of flows with finite-rate condensation and evaporation. Below, the basic approach is further discussed and the results are summarized.

Fluid Model

The flow of a two-phase fluid such as that found in a combustion-driven wind tunnel is described by a set of equations similar to the Navier-Stokes equations. This equation set is expanded to take into account the formation of water droplets, their growth, and possible evaporation. Additionally, the water droplets may have different velocities and temperatures than the gas phase. Thus, separate energy and momentum equations must be solved to determine these quantities. The governing equations for a two-dimensional flow may be written in conservation-law form as

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = W$$

Where U is the vector of conserved quantities and F and G are the flux vectors in the x and y directions. W is the source vector which represents the rate of transfer of mass, momentum, and energy between the gas phase and the liquid phase. For the case where there is assumed to be a single droplet size, U is

$$U = \left(\rho, \rho u, \rho v, E, \rho_w, \rho_w u_w, \rho_w v_w, E_w \right)'$$

where the quantities with subscript w denote the density, momentum, and energy of the water phase. The flux vector in the x direction is

$$F = \left(\rho u, \rho u^2 + p + \tau_{xx}, \rho uv + \tau_{xy}, (E + p)u + u\tau_{xx} + v\tau_{xy} + q_x, \rho_w u_w, \rho_w u_w^2, \rho_w u_w v_w, E_w u_w \right)'$$

The source vector, W , must be modeled to represent the rate of mass, momentum, and energy transfer between the gas phase and the liquid phase. For example, if the gas is condensing, there is a rate of liquid formation, which would tend to increase the density of the liquid phase, ρ_w , and decrease the density of the gas phase, ρ . Likewise, if the fluid particles have a different speed than the gas, there is a drag force acting on the liquid droplets which will tend to increase or decrease their momentum. This is represented by a source of liquid phase momentum and a sink of gas-phase momentum. There would be similar source and sink terms for the water and gas-phase energies.

We can relate the energy of the gas, E , and of the water, E_w , to the temperatures of the mixture.

$$E = \rho c_v T + \frac{1}{2} \rho (u^2 + v^2)$$

$$E_w = \rho_w c_{vw} T_w + \frac{1}{2} \rho_w (u_w^2 + v_w^2) + \rho_w h_w^\circ$$

where h_w° is the heat of formation of the water. The pressure of the gas is obtained from the perfect gas relation. The specific heat of the mixture, c_v , will depend on the amount of carrier gas and vaporized water present. With suitable expressions for the shear stresses and heat fluxes, and the appropriate models for the source vector, this is a closed set of equations.

The mass and energy source terms that appear in the source vector are derived from those developed by Young⁴ and extended by Erickson *et al*.² The momentum transfer term would be modeled using the expression for the drag coefficient⁵

$$C_D = K_D C_{D\text{Stokes}} = K_D \frac{24}{Re}$$

$$K_D = \frac{(1 + 0.15Re^{0.687})(1 + e^{-0.427/\mathcal{M}^{4.63} - 3.0/Re^{0.88}})}{1 + (\mathcal{M}/Re)(3.82 + 1.28e^{-1.25Re/\mathcal{M}})}$$

where Re_r and \mathcal{M} are the Reynolds and Mach numbers based on the relative velocity between the gas and liquid phases. From this, we may determine the drag force acting on a particle, and consequently, the momentum source term.

The above discussion is for the simple case where it is assumed that there is a single size of particle. However, in a hypersonic flow where condensation occurs, there will be a multitude of particle sizes. This distribution is represented using a series of “classes” of predetermined size. For example, we may assume that there are four possible sizes of particles, say 0 to 1 nanometer, 1 to 2 nanometers, 2 to 4 nanometers, and 4 to 10 nanometers (the choice of the classes and the size distribution is arbitrary). Mass, momentum, and energy would be transferred between these different classes and between the gas phase. Thus, for example, during the onset of condensation where particles are formed at a small size, some mass is fed into the smallest class. Then further condensation, and possibly evaporation occurs, increasing or decreasing the amount of water in the different classes. The mass in each particle class will change according to the local flow conditions. The number of classes and their spacing must be chosen appropriately for each problem. The finite-rate exchange terms that represent these processes were developed based on the work of Young⁴ and Erickson *et al*.² They are discussed in more detail in the enclosed paper.

Numerical Method

A newly-developed implicit finite-volume technique was used to solve the governing

equations. This method is based on the LU-SGS scheme of Yoon and Jameson⁶. It has been shown to be very efficient for inviscid flows with source terms such as those considered here⁷. The method was modified to handle the two-phase flow, and these changes are discussed in detail in the attached paper. This method yields converged solutions to the very stiff conservation equations. Typical run times and convergence properties are discussed in the enclosed paper.

Computational Results

Two types of flows have been studied with the newly-developed computational approach. The flow in the NASA Langley 8' High Temperature Tunnel nozzle has been simulated. At this point, no viscous effects have been included, however the results are in qualitative agreement with previous calculations and experiments. The condensation occurs very suddenly at about the 8 m point in the nozzle. This causes a rise in the pressure and temperature and a drop in the Mach number. These results are presented in detail in the enclosed paper. The second flow studied is the hypersonic flow over a circular cylinder. In this case, particles are introduced in the free-stream and then interact with the flow in the stagnation region of the cylinder. These calculations were performed to determine how much effect the presence of the particles has on testing bodies in a two-phase hypersonic flow. For the conditions chosen, most of the particles evaporate very quickly behind the bow shock wave, lowering the temperature in the stagnation region. For other conditions, this effect may be more prominent and may have a larger effect the flow. These results are also discussed in detail in the enclosed paper.

The computational method has been tested and used to compute several flows relevant to the flow in the NASA Langley 8'HTT. The method is still in development, but it shows promise to be used for the quantitative analysis of hypersonic flows with finite-rate condensation and evaporation of water.

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